Development and Testing of a New Unresolved Resonance Region Analysis Methodology

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Outline

- Objective
- Advantages
- Resolved Resonance Region
- Implementation of RML Algorithm
  - Test Cases: Energy-Differential and Double-Differential XS's
- Unresolved Resonance Region
  - New Methodology
  - Example Probability Table
- NCSP Project Goals

Objective

- Develop an unresolved resonance region (URR) analysis methodology consistent with the methodology used in the resolved resonance region (RRR)
  - improve model fidelity for both reactor simulations and shielding problems
- Added bonus – Help achieve goal of updating AMPX code to modern language (C++)

Advantages

- Eliminates the restriction of the Single-Level Breit-Wigner approximation
  - Allows evaluator to choose the cross-section formalism
- New approach gives group-averaged cross sections or probability tables, can be used with both deterministic and stochastic codes
- Allows for more reactions to be treated, such as inelastic scattering
- No major change in the ENDF format needed

Resolved Resonance Region (RRR)

- Energy region where resonances can be distinguished by the measurement technique
- Each resonance:
  - Represents an excited state of the compound nucleus
    - Can be completely described by a set of parameters, such as the resonance energy E_0, spin J, orbital momentum l, total width Γ_t, neutron width Γ_n, and all other partial (reaction) widths Γ_x (radiative Γ_γ, fission Γ_f, etc.)
  - Resonance parameters can be fit to the data with relative ease (harder as resonances start to overlap)

RRR Cross Section Reconstruction

- Several formulations available, all generate cross sections from resonance parameters, all can be derived from general R-Matrix Theory
  - Single-Level Breit-Wigner (SLBW)
  - Multi-Level Breit-Wigner (MLBW)
  - Adler-Adler (AA)
  - Reich-Moore (RM)
  - R-Matrix Limited (RML)
- RM Approximation
  - only allows for one gamma channel – currently available in ENDF
- RML
  - Most general – can treat every channel explicitly
  - Need more ENDF evaluations

- Why R-Matrix Limited Approximation?
  - Closest to full R-Matrix (too complex)
  - Treats capture channels in an aggregate manner, but:
    - Allows multiple inelastic channels and charged particle channels, like (n,α), (n,p), etc
    - All other reactions take into account channel-channel and level-level interference:

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_{\lambda} - E}\delta_{JJ'}$$

As opposed to SLBW (all interference effects ignored), MLBW (channel-channel interference ignored), Reich-Moore (no charged particles)

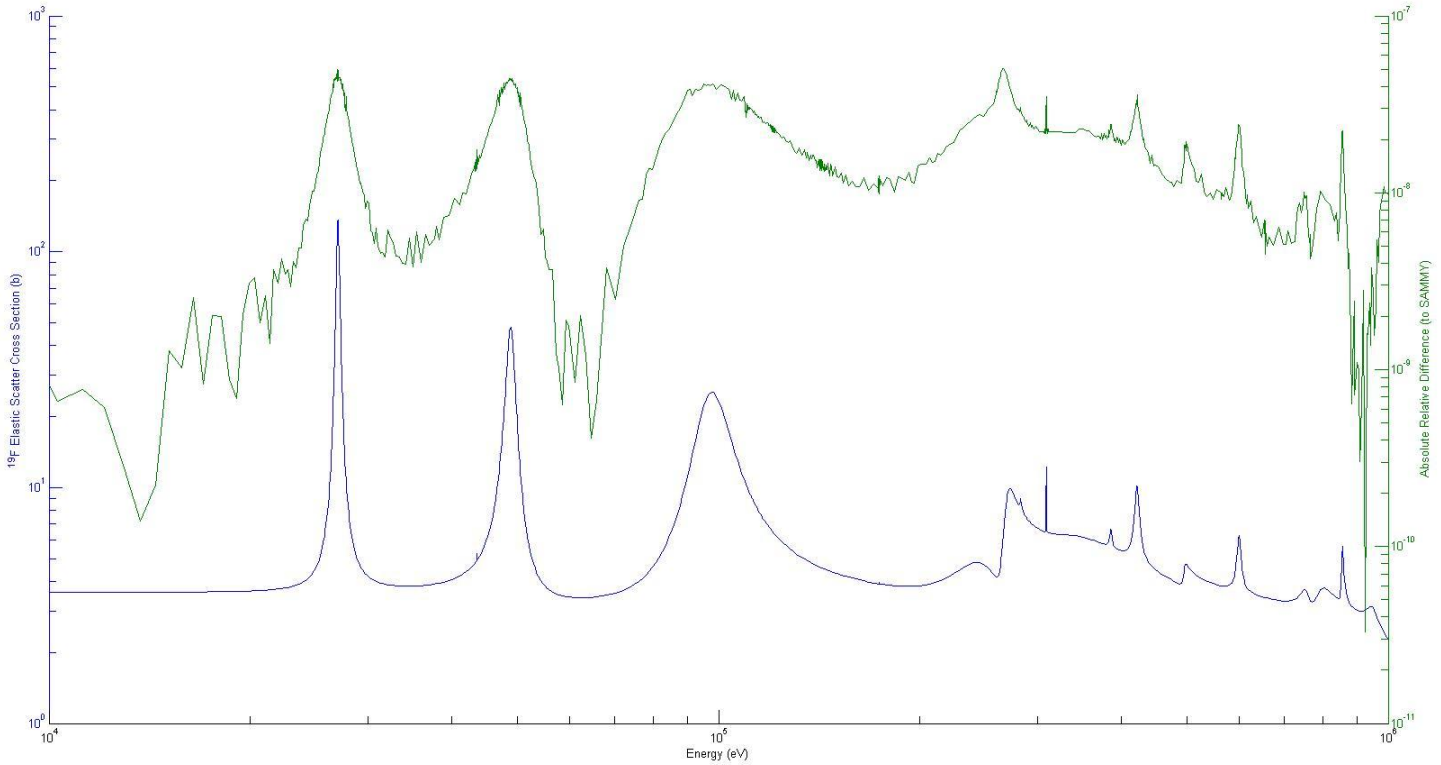
Implementation

- RML algorithm and new unresolved methodology are implemented in C++
  - Object-oriented programming
- Maintains modularity
  - Similar structure to original SAMRML routine
- Utilizes linear algebra package LAPACK
  - Takes advantage of complex data type

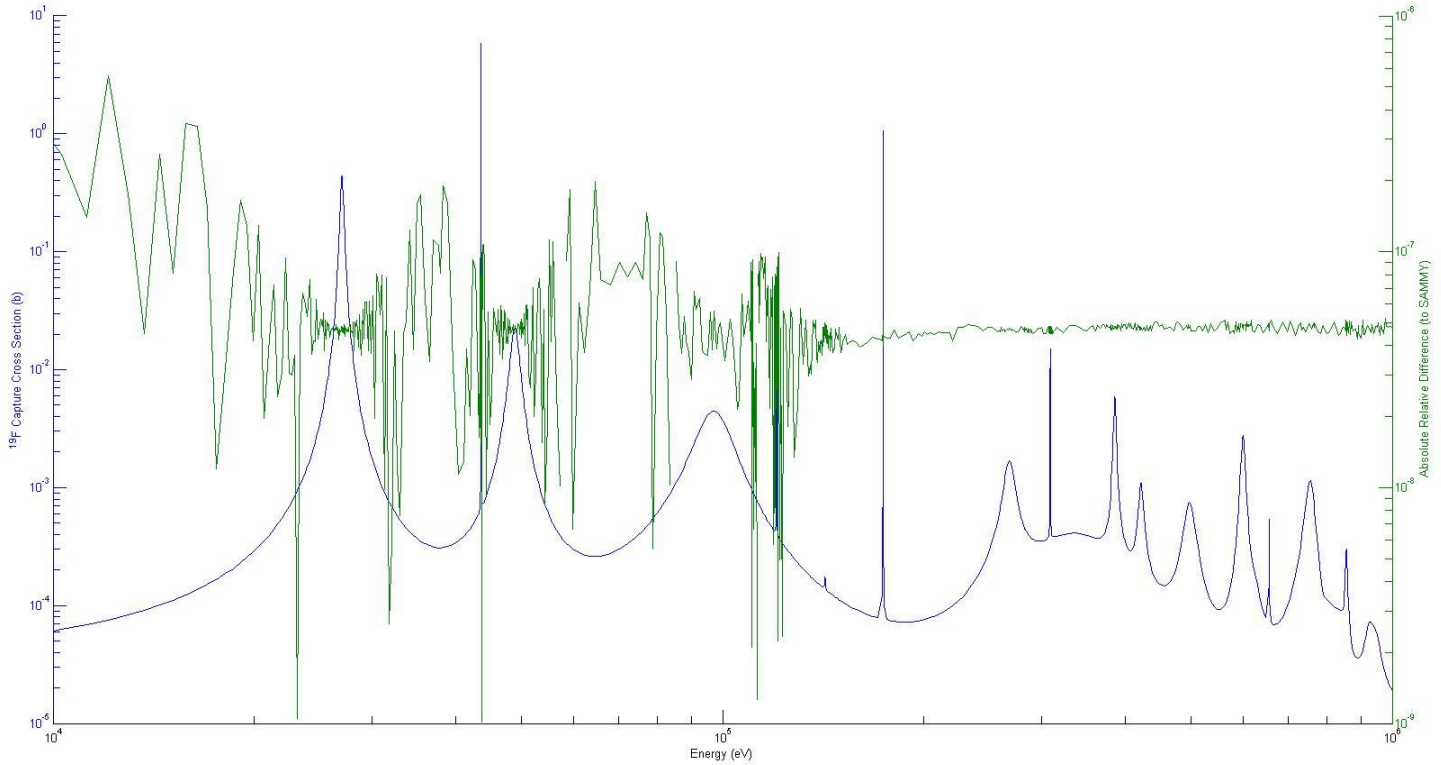
Test Cases

- Generated energy-differential and double-differential cross sections
  - Cross sections results verified by comparison with SAMMY
    - ^{19}F
      - Two inelastic channels
    - ^{16}O
      - (n,α), charged particle channel
    - Also verified ^{35}Cl and ^{56}Fe

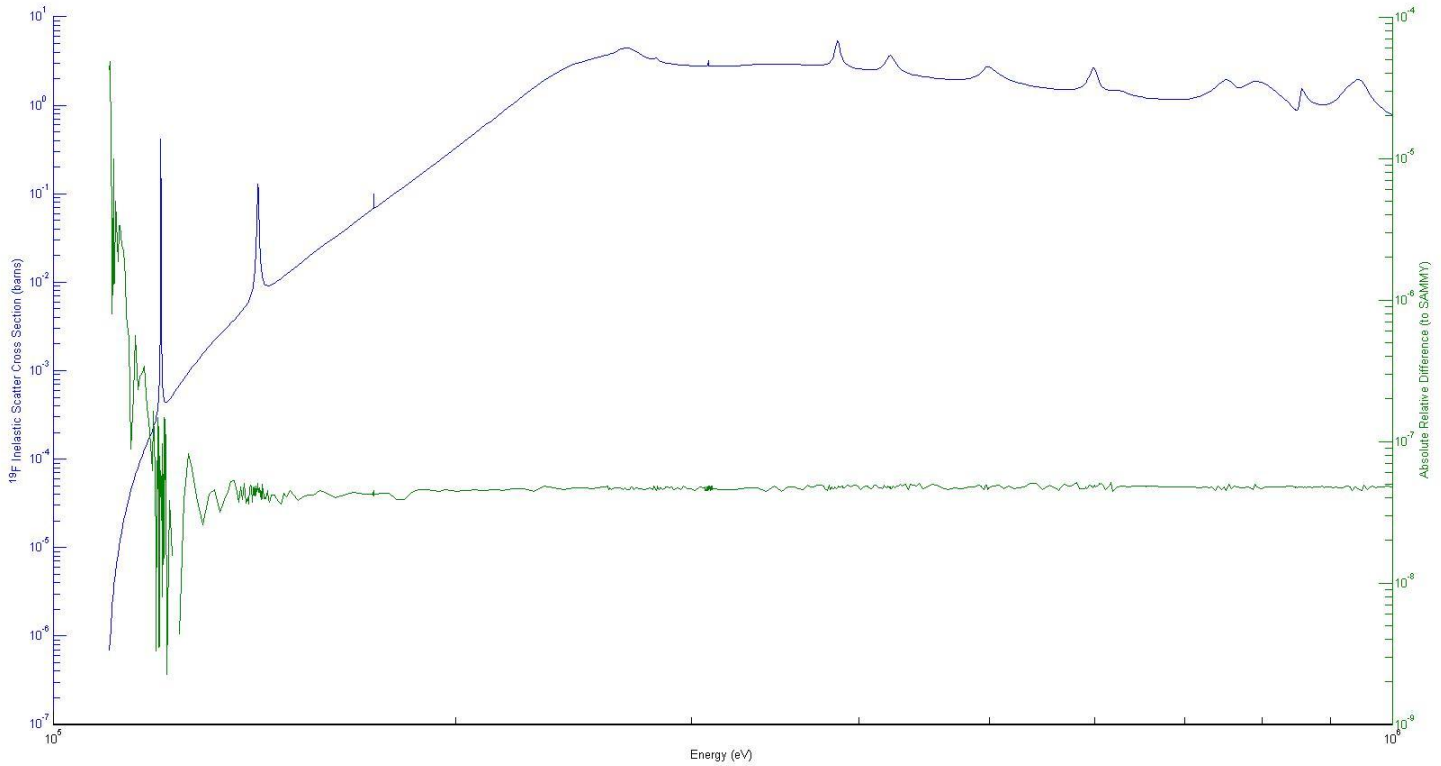
Energy-Differential Results - ^{19}F Elastic Scattering



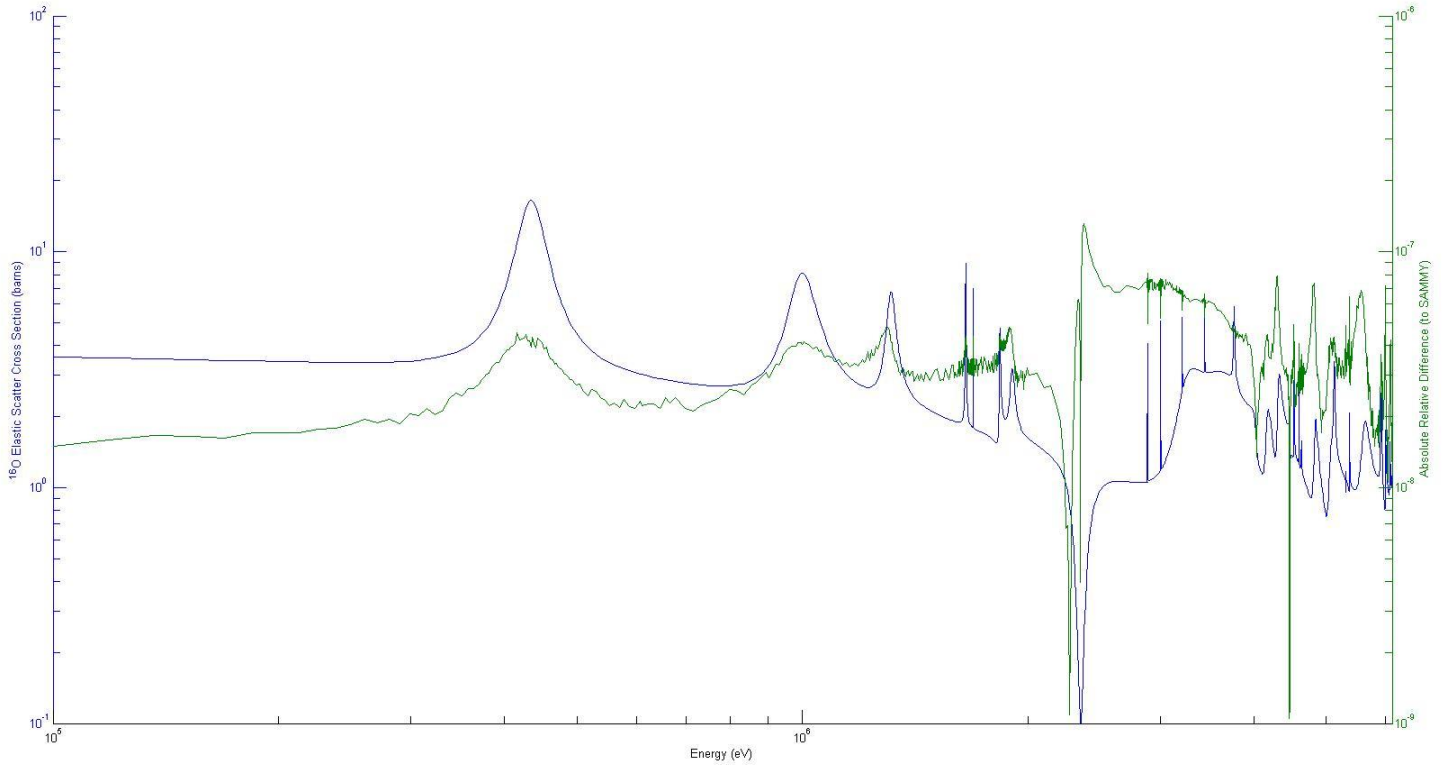
^{19}F Capture


^{19}F Capture Cross Section (b)
Absolute Relative Difference (to SAMMY)
Energy (eV)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{4}
10^{5}
10^{6}

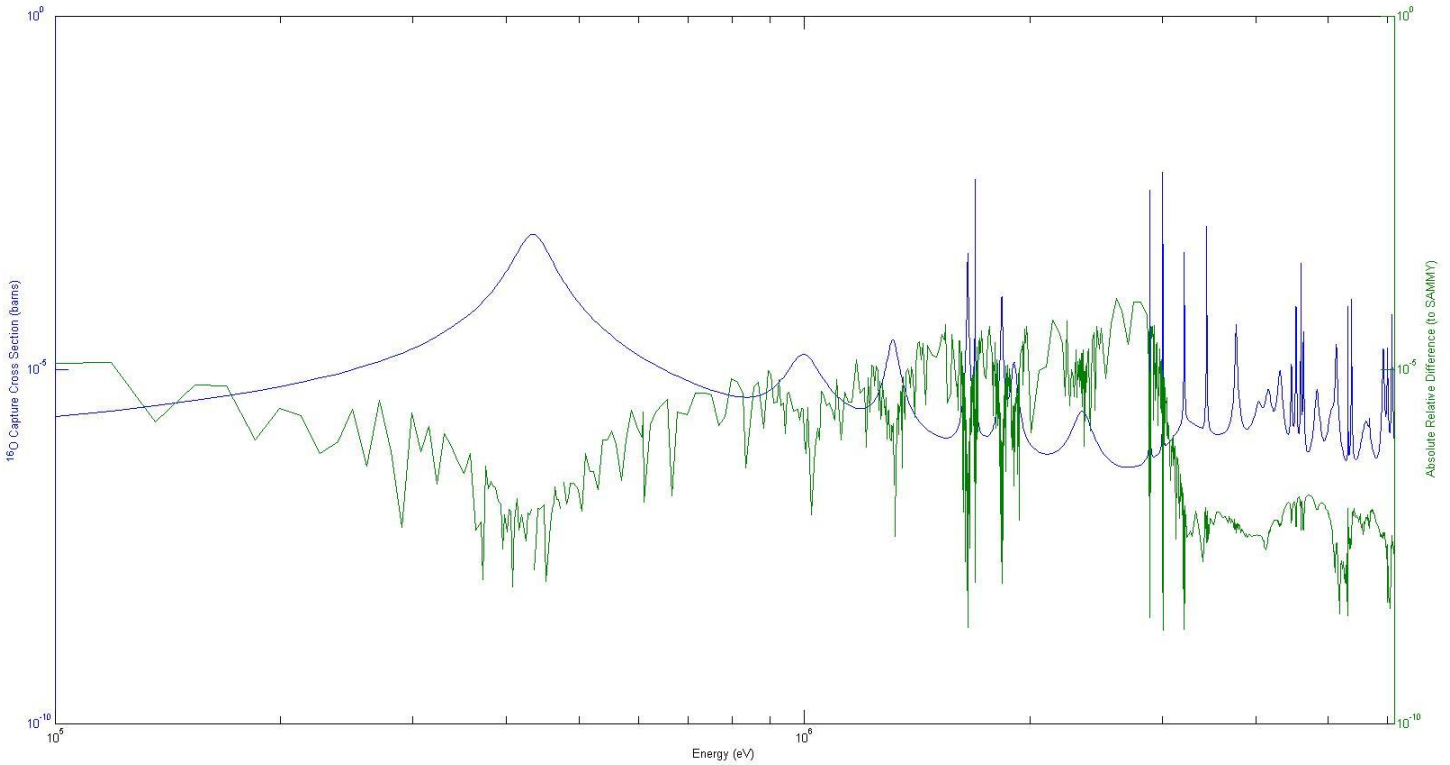
^{19}F Inelastic Scattering



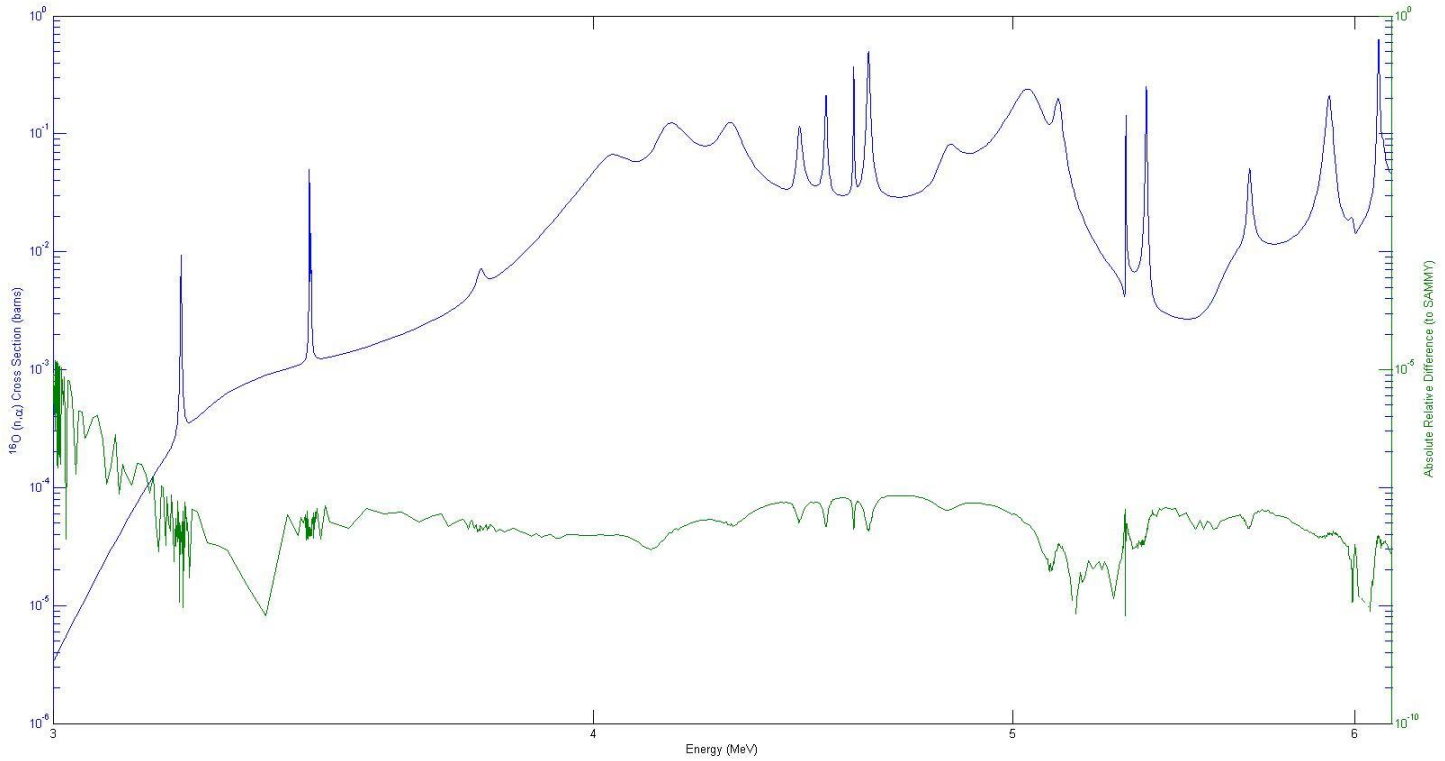
^{16}O Elastic Scattering



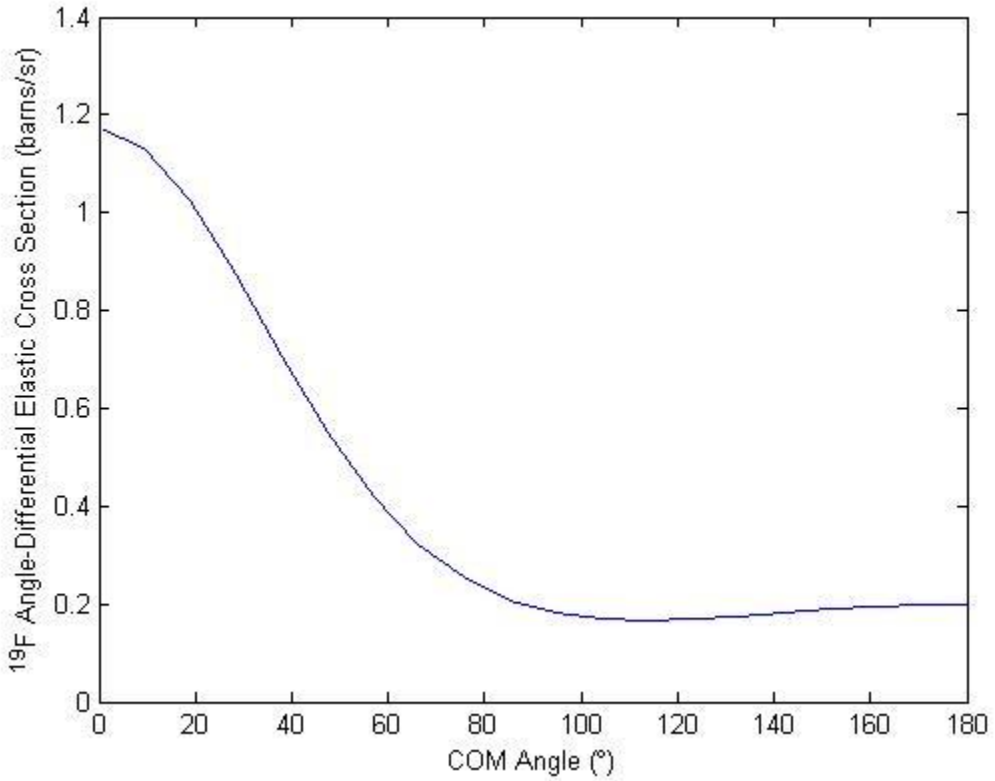
^{16}O Capture


10^{0}
10^{-5}
10^{-10}
^{16}O Capture Cross Section (barns)
Absolute Relative Difference (to SAMMY)
10^{5}
10^{6}
Energy (eV)

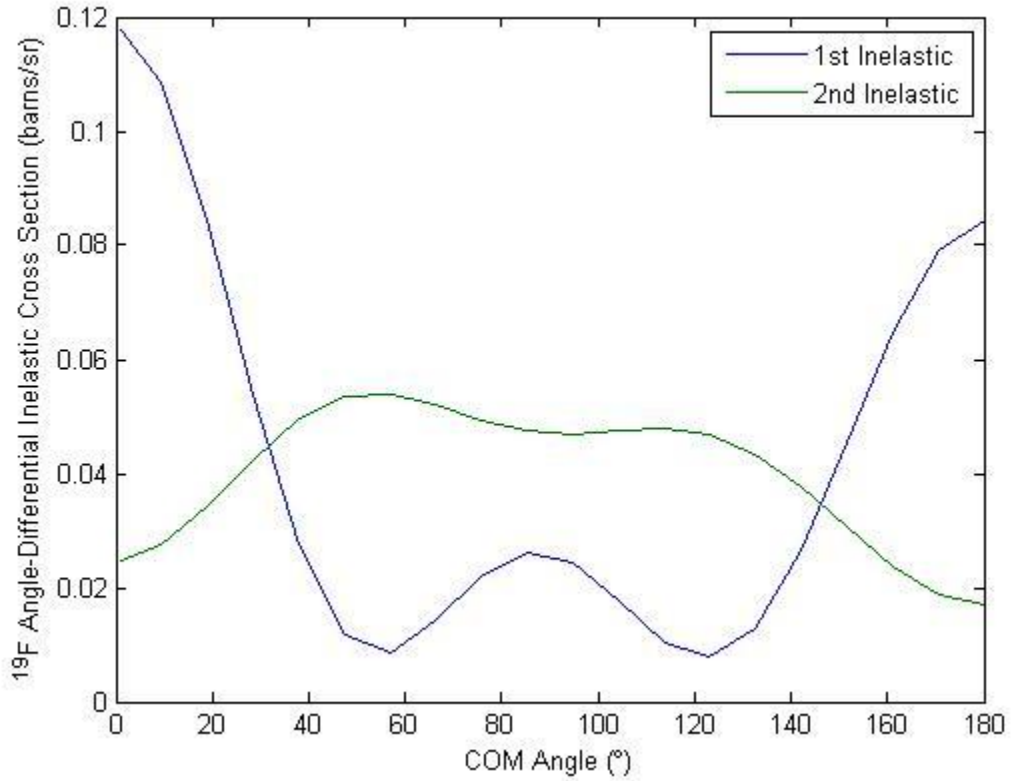
^{16}O – (n,α)


10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
^{16}O (n,α) Cross Section (barns)
3
4
5
6
Energy (MeV)
10^{0}
10^{-5}
10^{-10}
Absolute Relative Difference (to SAMMY)

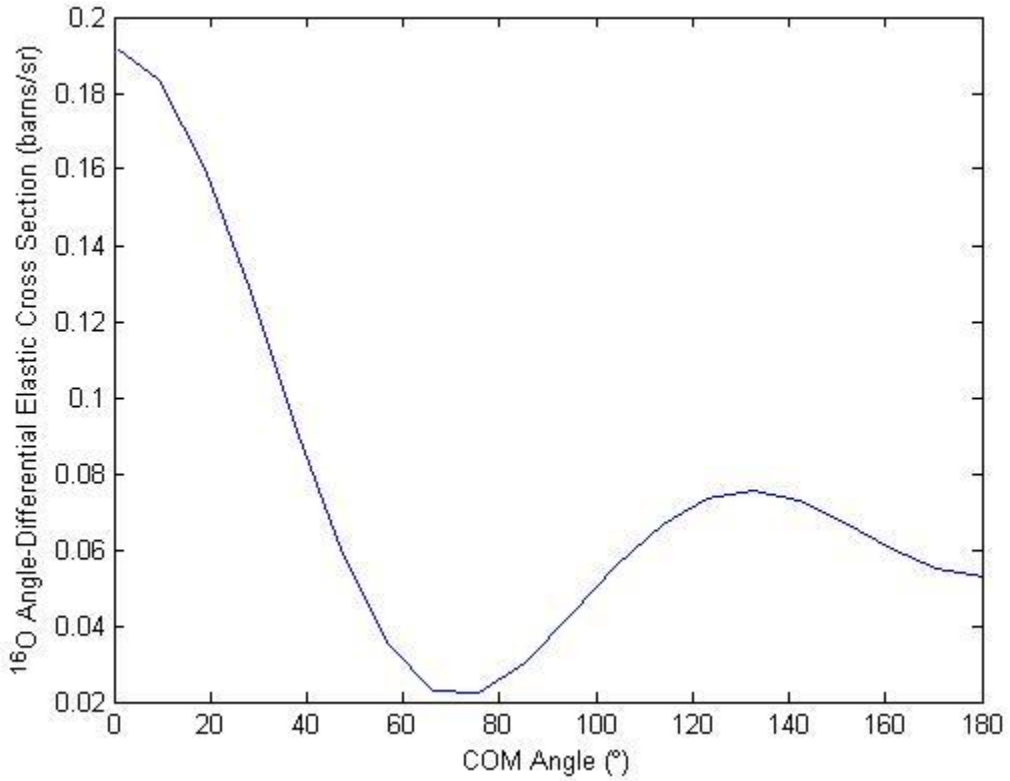
Double Differential Results- ^{19}F Elastic Scattering



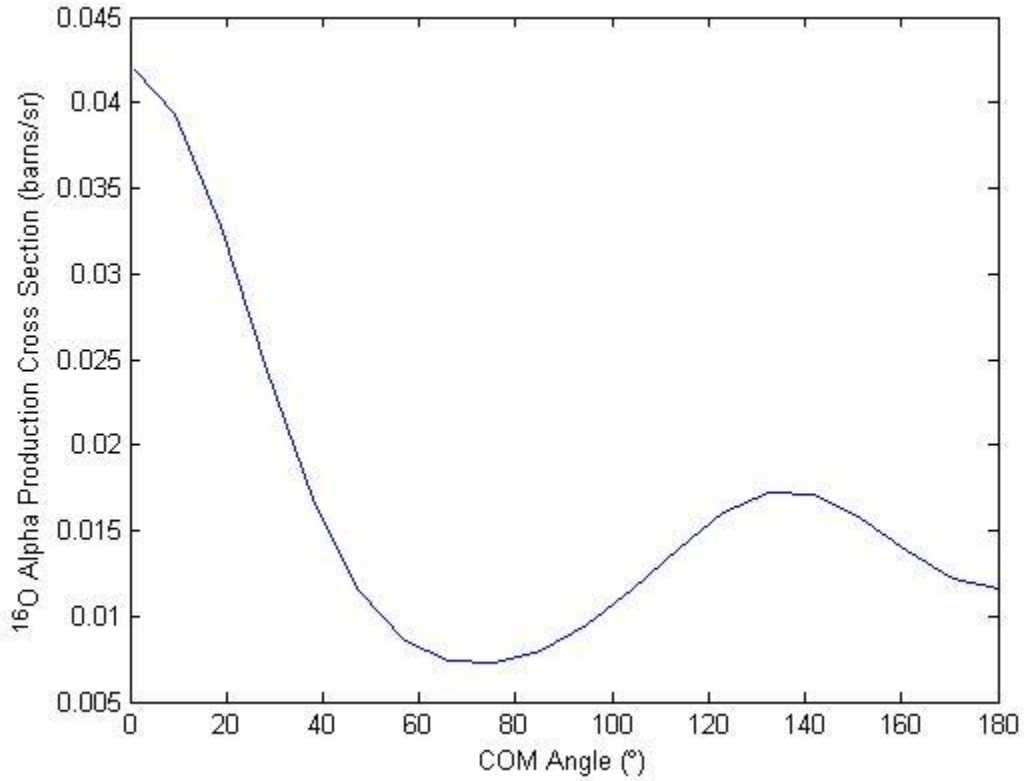
^{19}F Inelastic Scattering



^{16}O Elastic Scattering



^{16}O (n,α)


0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
20
40
60
80
100
120
140
160
180
16O Alpha Production Cross Section (barns/sr)
COM Angle (°)

Unresolved Resonance Region (URR)

- Still dominated by resonance structure! (same RRR physics apply)
  - Same resonance parameters, but since resonances have become indistinguishable, can only extract average values for the parameters
- Different from RRR in that it becomes impossible to discriminate between resonances

URR Cross Section Generation

- Only have average values, so XS's must be generated using a statistical sampling technique
  - Sample resonance level spacing to generate a pseudo-resonance ladder, for each resonance in the ladder, sample resonance width of each reaction, then calculate XS at reference energy
    - Used to generate probability table for XS sampling during neutronics calculation
- Currently, only one cross section formalism is available… Single-Level Breit-Wigner

New Methodology

- Resonance parameters are still sampled via a Monte Carlo routine from familiar distributions
  - However, instead of only placing resonances around the energy of reference, the new pseudo-resonance ladder generated spans the entire unresolved resonance range
- RML algorithm replaced by SLBW to calculate cross section values
  - Cross sections are calculated on an energy grid around the given (or chosen) energies of reference

- Gives the evaluator/user great amount of freedom
  - User can define the energy grid to use for each energy of reference which can be user defined, automatically chosen, or the same as the ones given in the ENDF file
  - Can generate a new ENDF file with different energies of reference than those given in the original file by extracting a new set of average parameters from the sampled ladders
  - Probability tables can be generated at different energies than those given in the ENDF file, and the table binning is also determined by the user (equi-probable, equi-spaced, etc.)

- Currently testing U-238
  - Tested to ensure that (within some statistical difference) the new ENDF file is the same as the old when the same energies of reference are used
  - Verified that the cross section values generated from each ladder and energy are correct (comparison with SAMMY results)
  - Generated probability tables with various binning options, can easily extract infinite dilution cross sections

- U-238, probability table at 45.1 keV without inelastic channel open

Bin	P(bin)	Total	Elastic	Capture	Inelastic	Non-elastic
1	0.20	6.08	5.95	0.13	0.00	0.13
2	0.20	9.33	9.28	0.05	0.00	0.05
3	0.20	10.42	10.36	0.06	0.00	0.06
4	0.20	11.89	11.77	0.12	0.00	0.12
5	0.20	26.42	24.92	1.50	0.00	1.50

- Still at 45.1 keV with channel open

Bin	P(bin)	Total	Elastic	Capture	Inelastic	Non-elastic
1	0.20	6.11	5.98	0.12	0.006	0.13
2	0.20	9.33	9.28	0.04	0.005	0.05
3	0.20	10.41	10.35	0.05	0.007	0.06
4	0.20	11.91	11.78	0.11	0.013	0.13
5	0.20	26.01	24.55	1.38	0.070	1.45

- Next energy of reference, 50 keV, open in either case

Bin	Prob	Total	Elastic	Capture	Inelastic	Non-elastic
1	0.20	6.28	6.14	0.12	0.02	0.14
2	0.20	9.45	9.40	0.04	0.02	0.06
3	0.20	10.49	10.42	0.05	0.02	0.07
4	0.20	11.94	11.80	0.10	0.04	0.14
5	0.20	25.64	24.12	1.28	0.24	1.52

NCSP Project Goals

- The development and demonstration of the new URR formalism/methodology will be accomplished as described in the tasks below.
  a) Work on the quasi-resonance parameter evaluation for U-238 using the computer code SAMMY in URR (20 – 100 keV);
  b) Include total, capture, fission, elastic, inelastic cross sections in the evaluation;
  c) Use the R-matrix limited (RML) cross-section formalism as opposed to the SLBW;
  d) Calculate average cross section based on average on energy (Riemann) and on probability table (Lebesgue);
  e) Derive covariance data;
  f) Implement the new formalism in the AMPX code.

Future Work

- Select benchmark problems from the International Handbook of Evaluated Criticality Safety Benchmark Experiments and compare results between the old and new methodology
- Derive covariance data
- Refactor code
  - Provide access to other AMPX functionality

References

1. M. E. Dunn and L. C. Leal, "A Monte Carlo Approach to Calculate Probability Tables for the Unresolved Resonance Region Using the AMPX Cross-Section Processing System," Proceedings of the International Conference on Nuclear Data for Science and Technology, 2001.
2. J. M. BLATT and L. C. BIEDENHARN, "The Angular Distribution of Scattering and Reaction Cross Sections," *Rev. Mod. Phy.*, **24**, *4*, 258 (1952).
3. M. E. DUNN and N. M. GREENE, "*AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications*", Trans. Am. Nucl. Soc., 86, 118 (2002).
4. N. M. LARSON, "Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations," ORNL/TM-9179/R8, Oak Ridge National Laboratory, Oak Ridge, TN, USA (2008).
5. Cacuci, Dan G. *Handbook of Nuclear Engineering*. New York London: Springer, 2010.

Questions?